

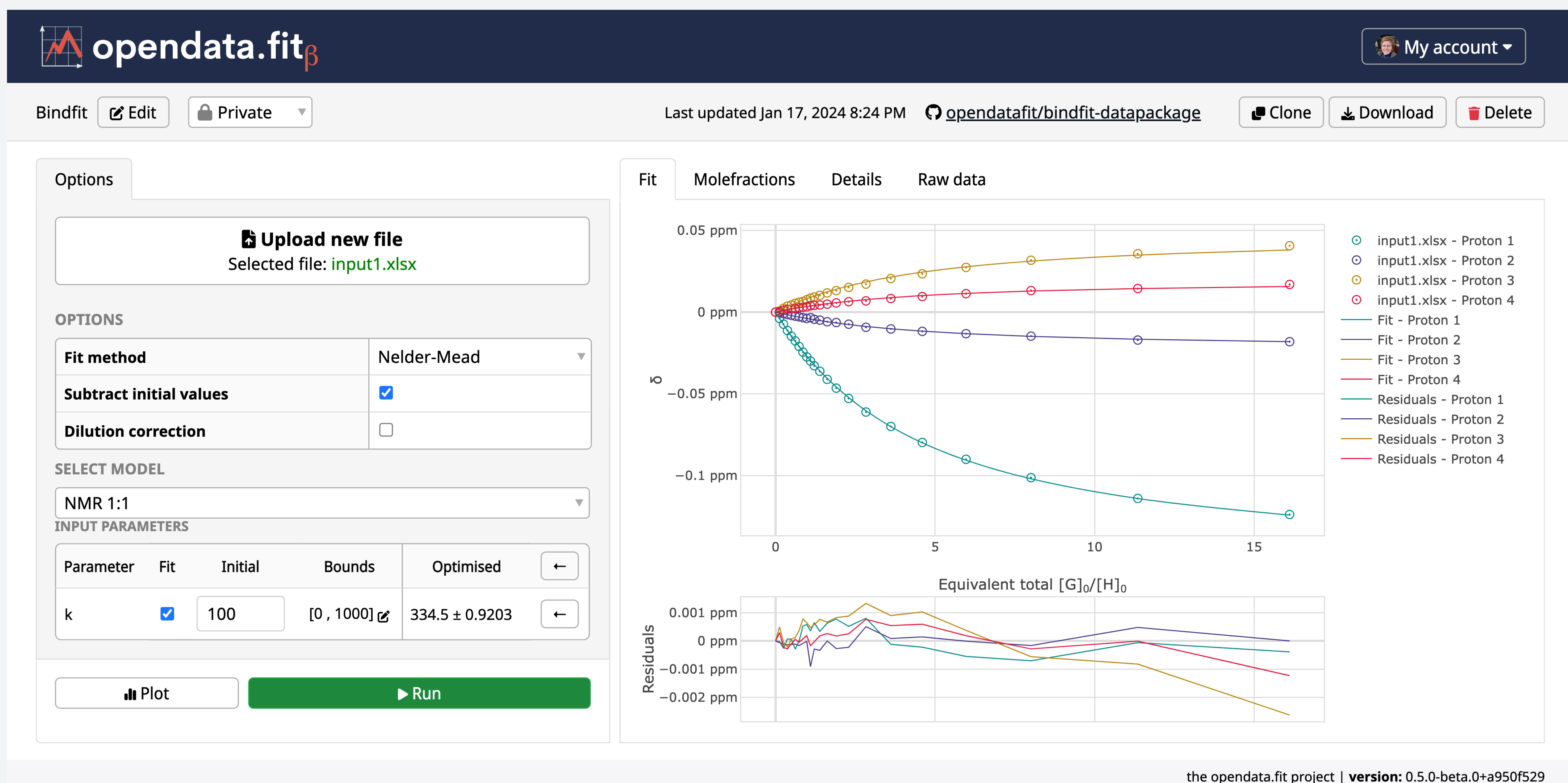
Introducing opendata.fit - the next iteration of supramolecular.org



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Example binding constant analysis in opendata.fit



What is opendata.fit?

opendata.fit is a data analysis platform that automatically captures data provenance and analysis history, making publishing reproducible workflows easy by citing a single URL.

It aims to provide users with a discipline-agnostic platform to manage scientific analysis workflows and datasets. It provides tooling to upload experiment data, run analysis algorithms in the cloud, visualise results, and finally publish workflows as citable entities.

Users will be able to choose from a library of existing workflows or write their own. It currently supports execution of Python-based analysis algorithms with plans to extend support to other common scientific computing languages.

supramolecular.org - Bindfit

Bindfit is a web-based binding constant fitting tool developed by the Thordarson group available at app.supramolecular.org/bindfit/. To date it has seen wide adoption with over 70 000 sessions and ~300 citations.

opendata.fit builds on this work, generalising the Bindfit concept to other data analysis applications.

Enabling reproducibility

Analysis workflows, datasets and input/output parameters vary widely between sub-specialties and can be difficult to track and publish in their entirety, resulting in difficulties with reproducibility.

opendata.fit provides tooling to improve reproducibility by encapsulating all of these elements into a JSON package format. Complete, reproducible workflows can then be easily published by citing an opendata.fit URL or attaching the datapackage directly.

Datapackages

Workflows in opendata.fit are packaged into a JSON package format called a datapackage.

Each datapackage is a complete, portable record of a workflow including datasets, algorithms, analysis process, input and output parameters, and user interface elements.

An example datapackage encapsulating the Bindfit workflow shown above is published on GitHub at the link below:
github.com/opendatafit/bindfit-datapackage

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